PROJECT NUMBER: 0008
PROJECT TITLE: CAD - Computer Technology
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PERIOD COVERED: June, 1989

I. Chemical Analysis Lab System

A. **Objective**: Develop a lab support environment for the Chemical Analysis Section including instrument support, sample receiving support, data reporting, and accounting.

B. **Results**: Version 1 of the Chemical Analysis Laboratory Support project was completed in May. This version's official release was accompanied by the creation of a release copy of the software, the deinstallation of the HP/1000 LIMS system and a final meeting with the Chemical Analysis Support team. This system, conceptually patterned after the current CTSD laboratory support system and providing a complete set of workstation/host cooperative systems, delivers enhanced capabilities including instrument run independence from a host environment, a standard style of supporting laboratory data and a consistent tool set for data control, editing, reduction and reporting. This system has made reported data available to high level analysis tools like RS/1 through electronic data transfer and direct interaction with a database of finished data.

This product provides the Chemical Analysis section with increased performance options, reliability and storage capacity while eliminating the obsolete HP 1000 system. The system is fully supported by the Computer Applications Division allowing for ease of modification and enhancement. The database design allows for flexibility in data retrieval and presentation. Its modular design accomodates the ability to add additional instrumentation with minimal software effort. Also, many of the concepts and development work done here are directly applicable to the modernization of the CTSD laboratory support system.

The current release includes the following features:

- Inhouse utilities provide Sample Receiving request logging, test specification, and label support under the Freeform database/screen tool and the ShareBase database platform.
- Worklists are generated on the host, downloaded to the instrument workstation and used to schedule testing. Results are reported locally. Approved results are uploaded to the hosts and incorporated into the ShareBase database.
- Design features of the system allow for instrument workstations to be run independently from a host computer. [New]

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- PC instrument workstations interact with tecnicians and with instruments to collect test results. IBM PC/XT microcomputers and in-house Microsoft Quick Basic utilities are used for gravimetric analyses. IBM PC/AT-compatibles and PE Nelson chromatography systems are used for the chromatographic and the continuous flow analyses. Results from these instrument workstations are concentrated on a central host using PC/NFS over ethernet. [New]
- Data storage is provided in an environment conducive to editing, screening, reporting and approving.
- Final data reports are automatically generated at the conclusion of the entry of data values. [New]
- Data Reporting and distribution is provided via electronic mail as requested. [New]
- Finished data is distributed to a long-term storage database. RPL procedures allow authorized personnel to extract this ShareBase data into RS/1. [New]
- An electronic accounting system has been established for tracking sample/test volume in the Chemical Analysis section. [New]

C. **Plans**: Requested enhancements for the current system will be handled via the project request system and incorporated on a prioritized and scheduled basis in a formal release cycle.

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